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Supporting Information

SUPPORTING
INFORMATIONConformational Complexity of Succinic Acid and Its Monoanion in the Gas
Phase and in Solution: Ab Initio Calculations and Monte Carlo SimulationsDaniel J. Price,[†] John D. Roberts,[‡] and William L. Jorgensen^{*,†}

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Supplementary Table 1. OPLS-AA Non-Bonded Parameters for Carboxylic Acids and
Carboxylate Anions

Atom	q, e	σ , Å	ϵ , kcal/mol
Acids			
C	0.520	3.750	0.105
O	-0.440	2.960	0.210
OH	-0.530	3.000	0.170
HO	0.450	0.000	0.000
HC	0.060	2.500	0.030
CT	a	3.500	0.066
Carboxylates			
C	0.700	3.750	0.105
O	-0.800	2.960	0.210
HC	0.060	2.500	0.030
α -CT	b	3.500	0.066
CT	a	3.500	0.066

^a Assigned to make the CH_n group neutral. ^b Assigned to make the charge on the α -CH_n
group = -0.10 e.

Supplementary Table 2. Bond Stretching and Angle Bending Parameters^a

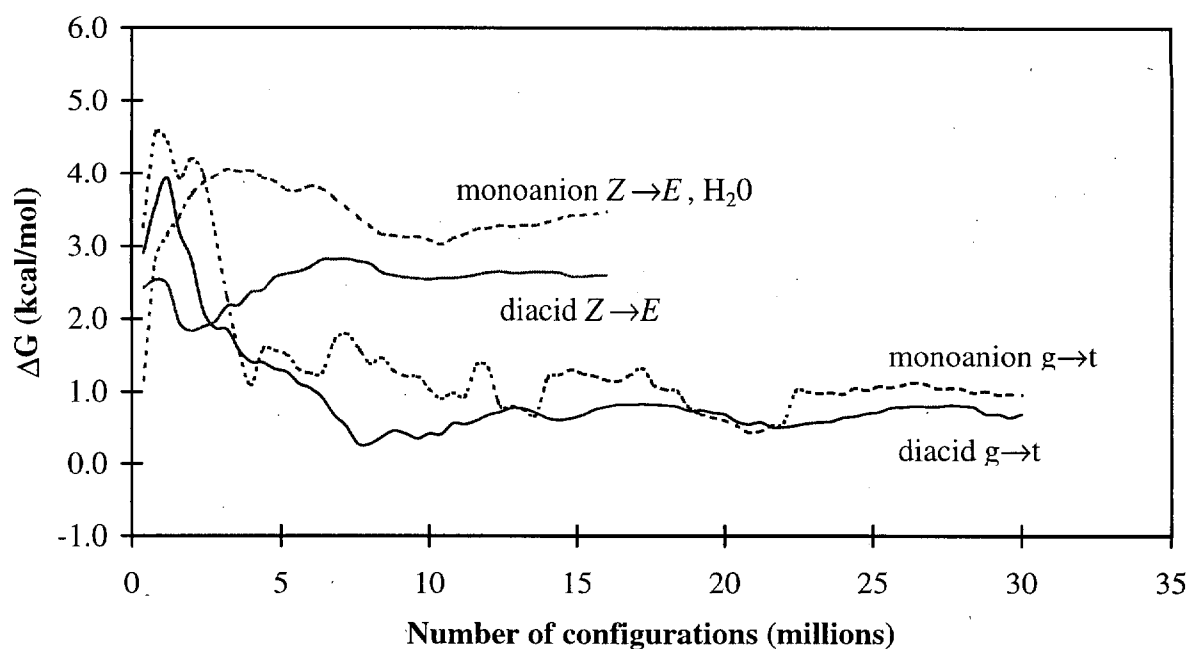
Bond or Angle	k	r ₀ or θ_0
CT-CT	268.0	1.529
CT-HC	340.0	1.090
C-CT	317.0	1.522
C-O	570.0	1.229
C-OH	450.0	1.364
OH-HO	553.0	0.945
C-CT-CT	63.0	111.1
C-CT-HC	35.0	109.5
C-OH-HO	35.0	113.0
CT-C-O	80.0	120.4
CT-C-OH	70.0	108.0
CT-CT-HC	37.5	110.7
O-C-OH	80.0	121.0
O-C-O	80.0	126.0

^a For bonds, k in kcal/mol-Å², r₀ in Å. For angles, k in kcal/mol-rad², θ_0 in degree

Supplementary Table 3. OPLS-AA Torsional Parameters for Carboxylic Acids and Carboxylate Anions

Angle Type	V ₁ , kcal/mol	V ₂ , kcal/mol	V ₃ , kcal/mol
Acids & Carboxylates			
CT-C-OH-HO	3.000	4.900	0.000
O-C-OH-HO	0.000	4.900	0.000
HC-CT-C-O	0.000	0.000	0.000
HC-CT-C-OH	0.000	0.000	0.000
CT-CT-C-O	0.000	0.546	0.000
CT-CT-C-OH	1.000	0.546	0.450
HC-CT-CT-C	0.000	0.000	0.074
HC-CT-CT-HC ^a	0.000	0.000	0.318
HC-CT-CT-CT ^a	0.000	0.000	0.366
CT-CT-CT-CT ^a	1.740	-0.157	0.279
Monocarboxylates			
CT-CT-C-O	0.000	0.820	0.000
HC-CT-CT-C	0.000	0.000	-0.225
CT-CT-CT-C	-3.185	-0.825	0.493
1,2-Diacids			
CT-CT-C-O	-0.750	-0.550	-0.250
C-CT-CT-C	-0.550	0.000	1.000
1,2-Diacid Monoanions			
CT-C-OH-HO	3.200	4.900	0.000
CT-CT-C-O	-1.000	-1.900	-0.900
C-CT-CT-C	0.800	0.000	0.900

^a Standard alkane parameters (reference 11).



Supplementary Figure 1. Convergence of the Z to E and gauche to trans free energy changes from the FEP calculations. The abscissa records the number of Monte Carlo configurations during the averaging periods.

HF/6-31G* optimized structure of the ZsgsZ conformer of succinic acid in Gaussian Z-matrix format.

Gaussian Z-matrix ZsgsZ diprotic succinic acid MP2/6-311+G**//HF/6-31G*
E=-455.9529098 au

```

0 1
C
X 1      1.000000
X 2      1.000000  1      90.000000
C 1      1.520384  2      90.000000  3      0.000000
C 4      1.507496  1      112.095989  2      0.000000
O 5      1.188012  4      125.347101  1      11.052565
O 5      1.327427  4      111.927674  6      178.389509
C 1      1.507497  4      112.095967  5      69.166660
O 8      1.188012  1      125.347142  4      11.052062
O 8      1.327427  1      111.927652  9      178.390538
H 7      0.952416  5      108.290759  6      -1.132562
H 10     0.952416  8      108.290731  9      -1.132066
H 1      1.081912  4      111.439324  8      -121.734613
H 1      1.086127  4      110.431307  8      119.463402
H 4      1.086127  1      110.431277  5      119.463412
H 4      1.081912  1      111.439326  5      -121.734553

```

HF/6-31+G* optimized structure of the Ecgs conformer of succinate in Gaussian Z-matrix format.

Gaussian Z-matrix Ecgs succinate MP2/6-311+G**//HF/6-31+G* MP2
E=-455.4222834 au

```

0 1
C
X 1      1.000000
X 2      1.000000  1      90.000000
C 1      1.540236  2      90.000000  3      0.000000
C 4      1.521219  1      116.308174  2      0.000000
O 5      1.200654  4      121.572561  1      128.044945
O 5      1.306279  4      116.725532  6      178.879262
C 1      1.544473  4      115.943705  3      146.345245
O 8      1.223141  1      116.486398  4      148.686535
O 8      1.253989  1      115.816590  9      179.083587
H 7      0.990952  5      111.058290  6      181.250227
H 1      1.083663  4      108.865009  8      121.612331
H 1      1.089319  4      110.026112  8      237.673025
H 4      1.087456  1      109.215292  5      238.312146
H 4      1.082810  1      110.106546  5      120.446705

```